

Approach to Translational Equilibrium in a Rigid Sphere Gas

G. A. BRAD

Department of Aeronautical Engineering, University of Sydney,

Sydney, Australia

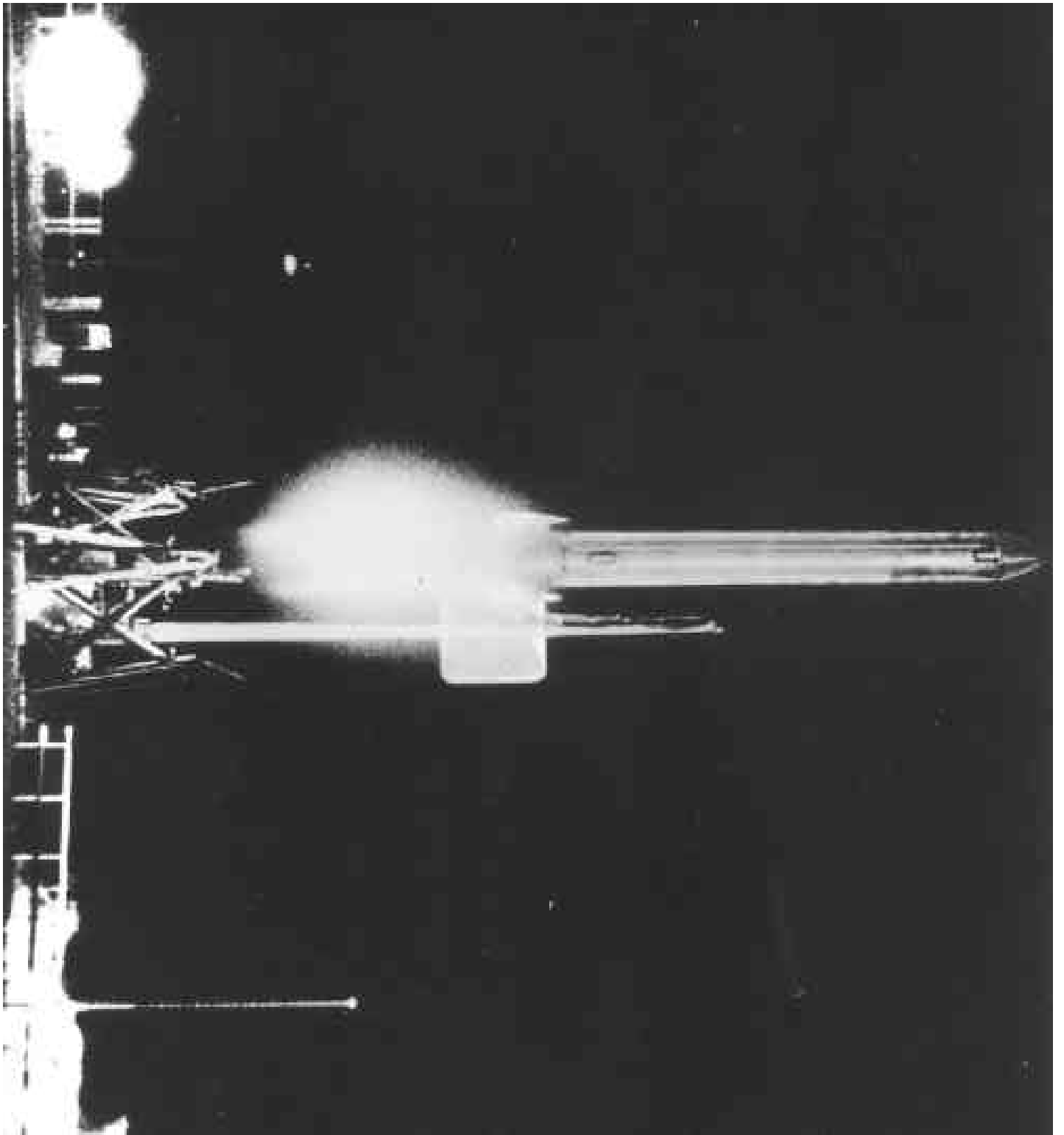
(Received 10 May 1963)

It is usually assumed that the translational degree of freedom in a gas reaches equilibrium in a time of the order of the mean collision time. Some confirmation of this has been supplied by Alder and Wainwright¹ who used their "molecular dynamic" method to determine the rate of approach to Maxwellian equilibrium of a set of molecules which all start with the same speed. This method effectively solves the simultaneous equations of all the molecules in a closed container and is valid for dense gases.

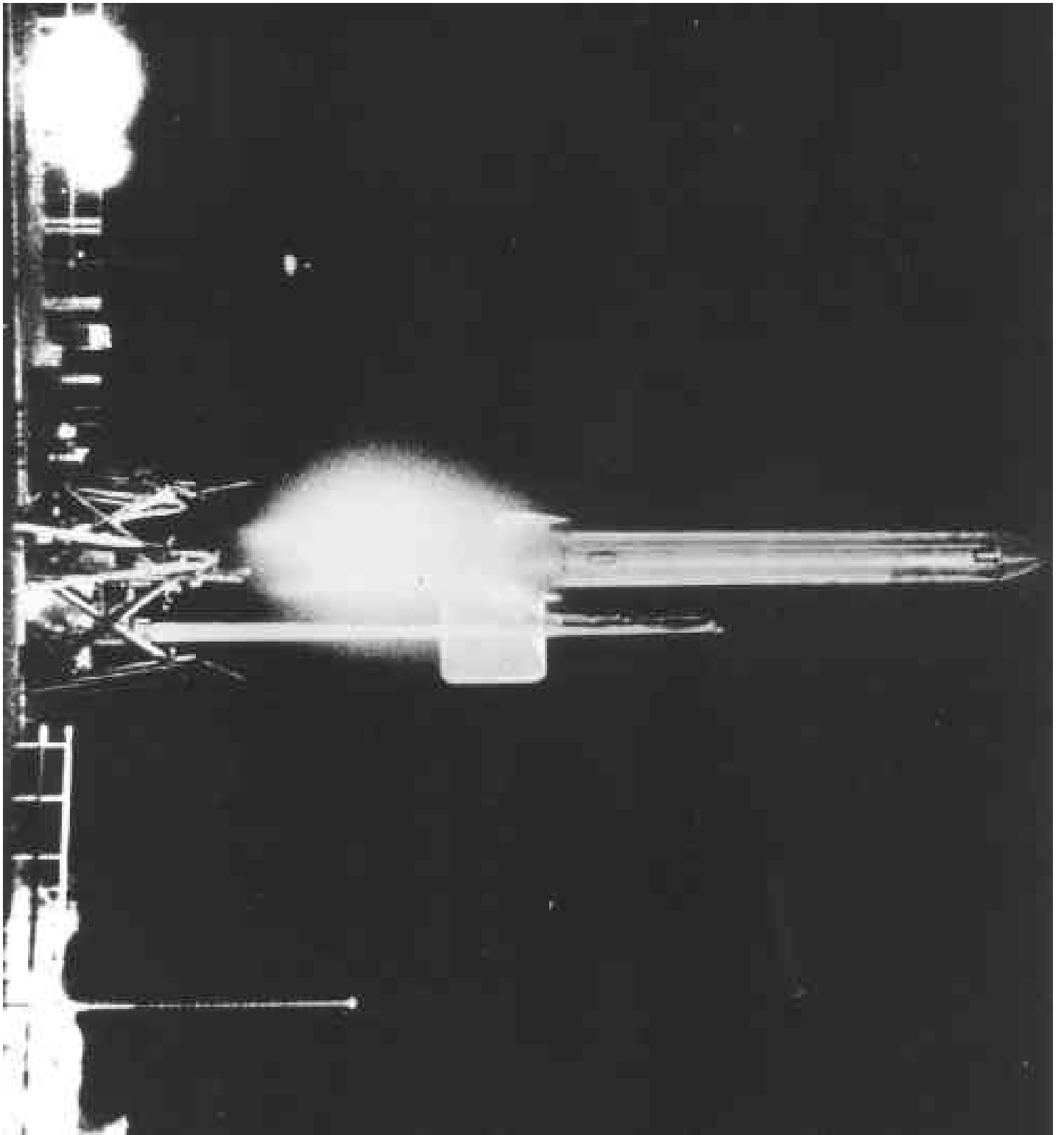
However, it makes great demands on computer time and storage capacity, and Alder and Wainwright were limited to 100 molecules which was an insufficient number to enable information to be gained on the rate of approach to equilibrium in the higher speed ranges of the distribution. The present note reports on an investigation of this problem

Using the Silliac digital computer in the University of Sydney, more than 30 000 collisions were computed per hour of computing time. The results quoted below are based on the mean of ten runs each involving 500 molecules. As a check on the accuracy of the Monte Carlo-type approach, the mean free path and the collision frequency were calculated by assigning the appropriate time interval to each collision. Figure 1 shows the behavior of the mean free path λ with the mean collision time (i.e. the time in which each molecule suffers an average of one collision). The six percent change in the mean free path from the Clausius value² for a constant-speed gas to the value for a Maxwellian gas is discernable. The collision frequency was also in excellent agreement with the theoretical value.

It was found that the general features of the Maxwellian distribution were established after about four collisions. For instance, Fig. 2 shows the fraction f of molecules with speeds between 0.9 and 1.1 times the root mean square speed v_r . This fraction is initially unity and, after collisions have started, it tends rapidly to its Maxwellian value of 0.1838. The lower speed ranges were filled from zero









THE ELECTRONIC COMPUTER

"SILLIAC"

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REPRINTED FROM

RAREFIED GAS DYNAMICS, VOLUME 1

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ACADEMIC PRESS INC., NEW YORK

Shock-Wave Structure in a Rigid Sphere Gas¹

G. A. BIRD²

Department of Mechanics of Fluids, University of Manchester, Manchester, England

Consideration is given to a gas composed of rigid sphere molecules, initially in thermal equilibrium between two infinite, plane, parallel and specularly reflecting walls. A Monte Carlo approach is used to study the shock wave which is formed when one wall impulsively acquires a uniform velocity towards the other. The method essentially consists of carrying out a "numerical experiment" with a model gas on a very fast computer. Shock wave density profiles are presented for shock Mach numbers 1.0 to 1.5.

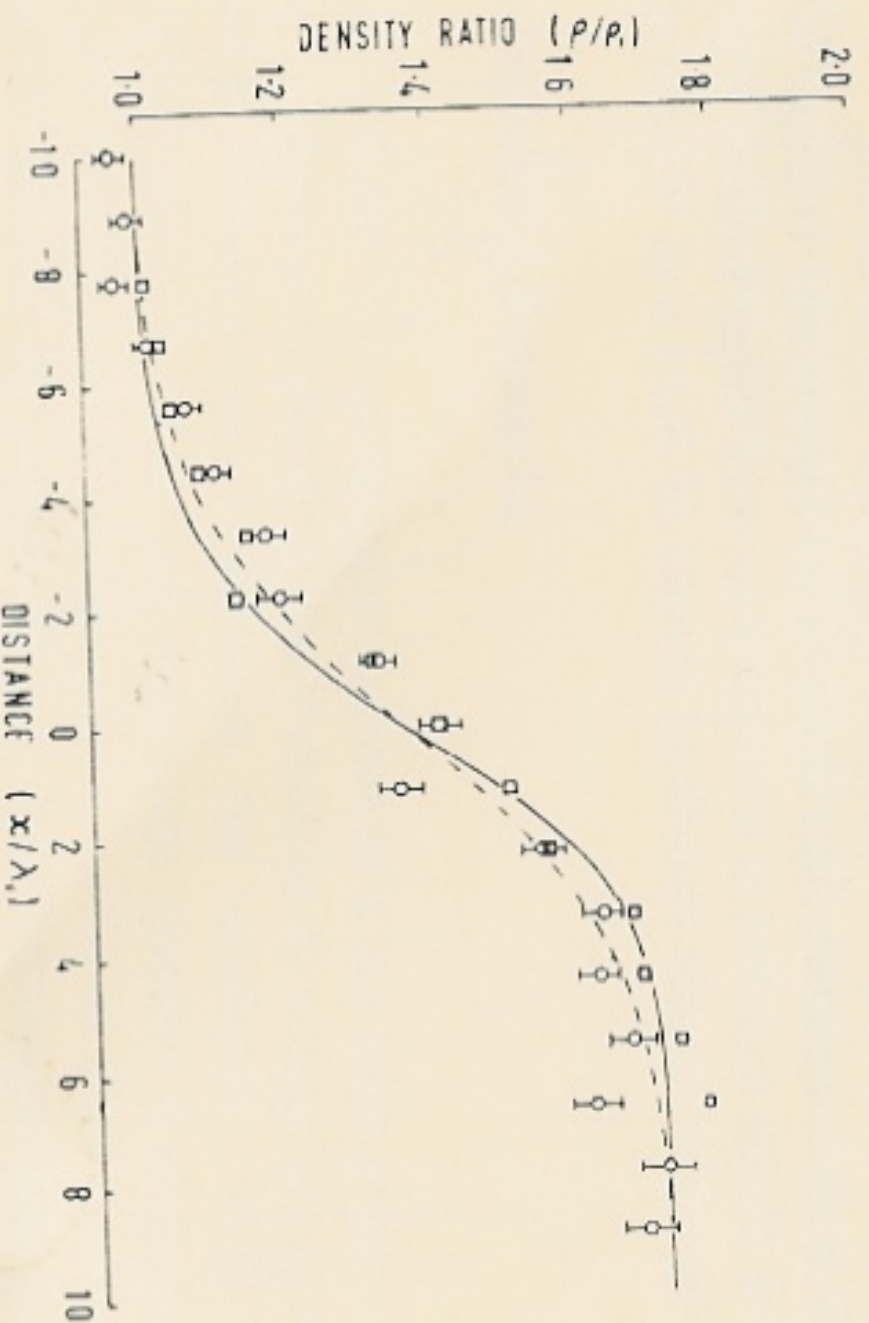


FIG. 1. Shock wave density profile for $M_s = 1.5$. Model gas, run 1, O, $\updownarrow \pm$ one standard deviation; run 2, \square ; Navier-Stokes, —; Mott-Smith, ---.

1964 – Lack of acceptance bordering on hostility

- **DSMC was an heuristic method that did not provide a solution to any equation, and certainly not of the Boltzmann equation.**
- **DSMC was too expensive and provided noisy results.**
- **DSMC provided results for contentious problems that were later verified by experimental studies.**
- **The DSMC procedures were shown to be consistent with the derivation of the Boltzmann equations.**
- **The procedures and molecular models were gradually improved and the “user community” grew to a significant size.**
- **Idealized DSMC procedures were shown to provide a solution of the Boltzmann equation.**
- **DSMC was shown, in some dense gas cases, to go beyond the Boltzmann model.**

2003–“DSMC is a solution of the Boltzmann equation”

**From: *Computational Gasdynamics*
C.B. Laney (Cambridge Univ. Press)**

The need for free and low-cost CFD software is greater than ever. Commercial CFD software costs an enormous amount - \$25,000 for a one-year lease for a single computer is typical.

Full-blown CFD software, free or not, typically requires new users to invest weeks or months to fully understand and use it properly. You should have a basis for confidence in a given code before making such a commitment.

CFD codes will give an answer to most problems when consistently and properly posed, but they require patience, practice, and expertise to produce a reasonable answer.



“A mathematician is a person who is more interested in the equations than in the flow.” (anon, circa 1950)

CFD appears, almost by definition, to be concerned only with the Navier-Stokes equations.

From the physical point of view, the derivation of the equations is more instructive than the form of the equations.

A gas is comprised of molecules and particle based methods should always be better than methods that assume the gas to be a continuous medium. The transport terms in the N-S equations are incomplete approximations.

If computers were faster by 20 orders of magnitude, Navier-Stokes based CFD would be obsolete.

Direct simulation methods are best developed for particle systems without reference to mathematical models such as the Boltzmann equation.

(Please write down the Boltzmann equation for a chemically reacting gas with line radiation and selective absorption!)

Simulation is unsteady and allows event-driven processes.

e.g. quantum vibration model with dissociation and radiation

In a collision with relative translational energy ε_t a molecule in vibrational state i has energy $\varepsilon_v = i k \Theta_v$ and the normalized probability of a post-collision vibrational state i^* is

$$P/P_{max} = [1 - i^* k \Theta_v / (\varepsilon_t + \varepsilon_v)]^{3/2 - \omega},$$

where k is the Boltzmann constant, Θ_v is the characteristic vibrational temperature, and ω is the viscosity-temperature index. The state i is stored for each vibrational mode of every molecule and the vibrational temperature of a mode is

$$T_{vib} = \Theta_v / \ln (1 + 1 / \langle i \rangle),$$

while the effective number of degrees of freedom of the mode is

$$\zeta_{vib} = 2 \langle i \rangle \ln (1 + 1 / \langle i \rangle).$$

Dissociation occurs if i^* is the state that leads to dissociation. The vibrational relaxation rate then sets the dissociation rate.

The Einstein coefficients set the probability of each bound-to-bound radiative transition over any time interval.